

Atom Elm Bonded To

1	C	2
2	C	1,3,4
3	O	2
4	C	2,5,6,7
5	C	4
6	C	4
7	C	4

Simplified

Connection Table

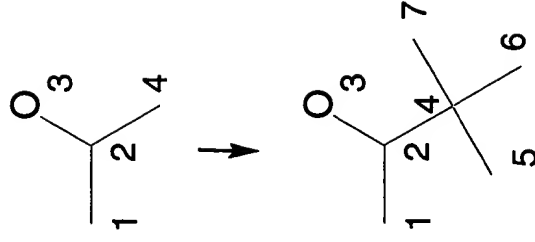
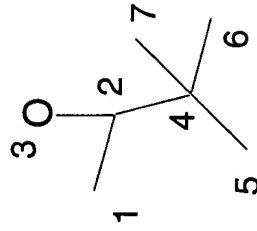
...and the molecule
it represents

FIG. 1A

(PRIOR ART)

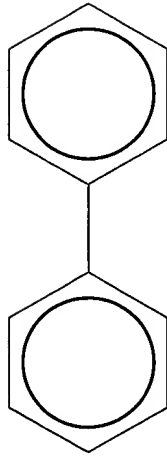
FIG. 1B

(PRIOR ART)

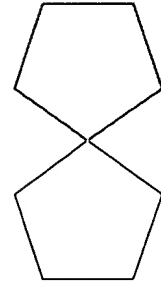


Resultant
molecule

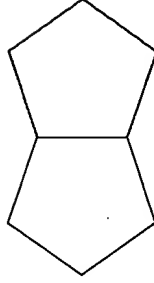
FIG. 1C



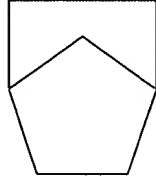
Two different ring systems are present



Spiro

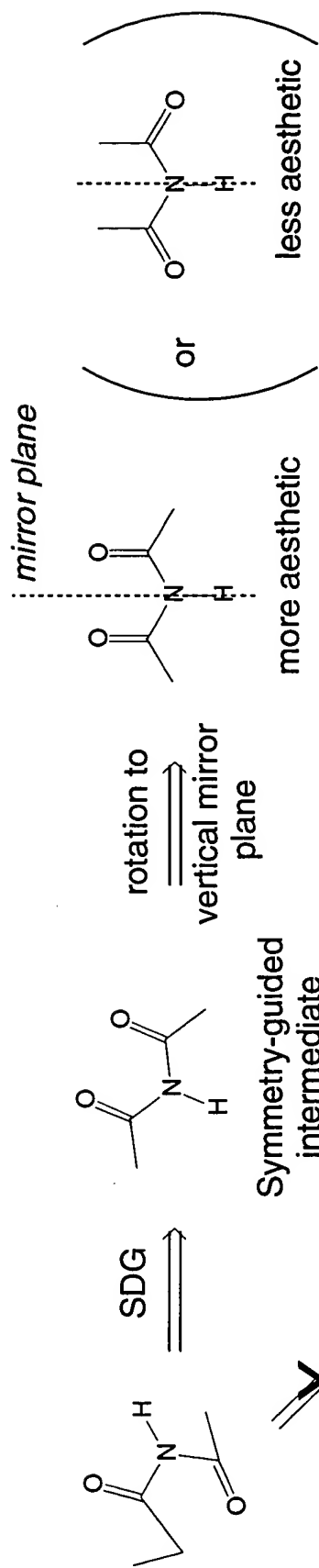


Fused

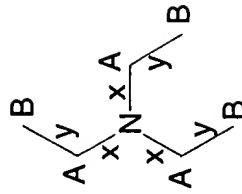
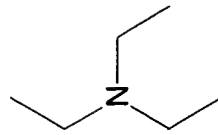


Bridged

FIG. 2
(prior art)



F16.3

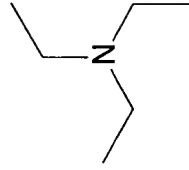
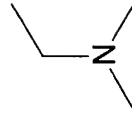
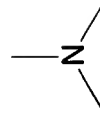


a. Given structure
(Starting coordinates
are irrelevant.)

b. Perceived symmetry.
Like letters indicate
equivalent atoms or bonds.
Symmetry is three-fold.

c. The pivot atom is
taken as the first
seed atom.

d. Place an
adjacent atom.

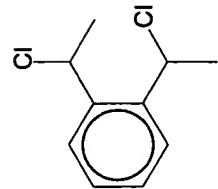


e. Place equivalent
atoms, with three-
fold symmetry

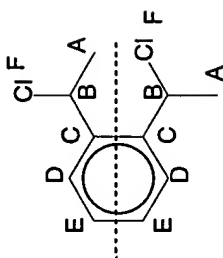
f. Place next
atom. (Direction
is arbitrary.)

g. Place equivalent
atoms, with three-
fold symmetry.

FIG. 4



a. Given structure
(Starting coordinates
are irrelevant.)



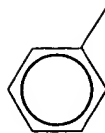
b. Perceived symmetry.
Like letters indicate
equivalent atoms.
Symmetry is reflection.



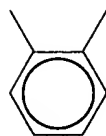
c. Deposit
first atom.



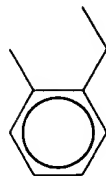
d. Because it is cyclic,
we deposit the whole
ring as one unit.



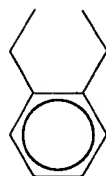
e. Place
next atom.



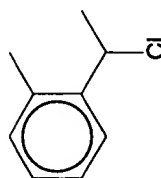
f. Place equivalent
atom, with reflectional
symmetry



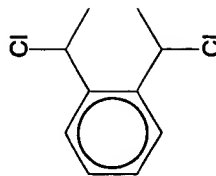
g. Place next
atom. (Direction
is arbitrary.)



h. Place equivalent
atom, with reflectional
symmetry.



i. Place next
atom.



j. Place equivalent
atom, with reflectional
symmetry.

Fig. 5

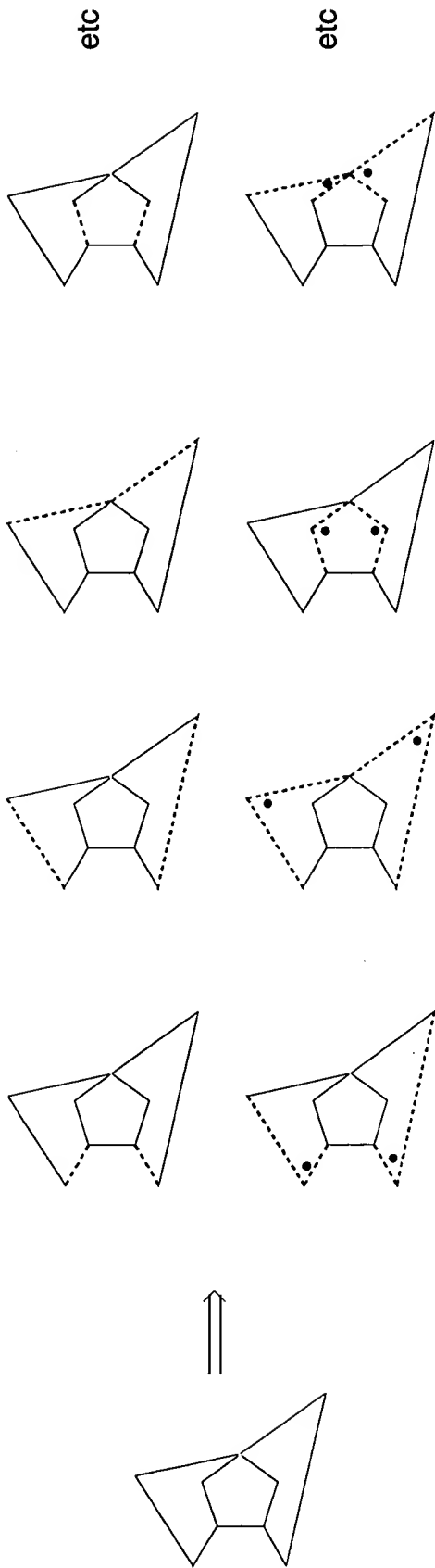


FIG. 6

FIG. 16.7 is a schematic diagram of a mechanical linkage system. The diagram shows a central pentagonal link (1) connected to four other links (2, 3, 4, 5) which form a closed loop. The links are connected at their vertices. The diagram illustrates the kinematic structure of the mechanism.

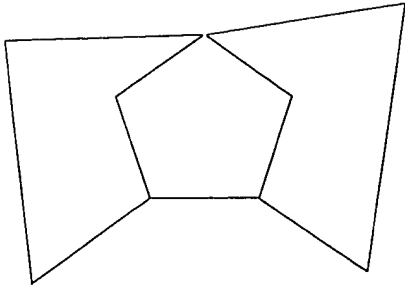
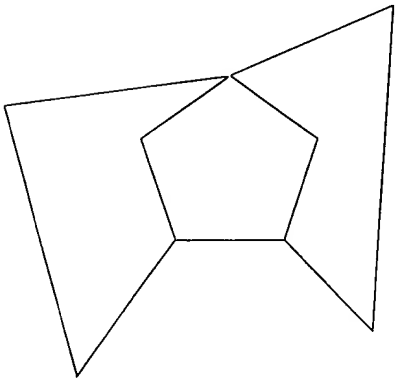
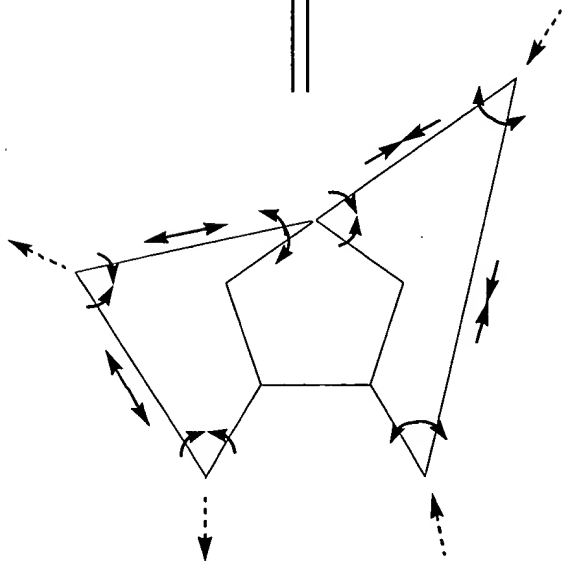
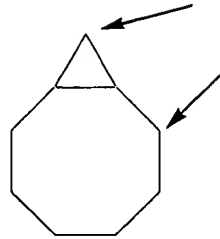
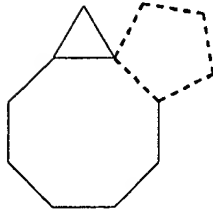


FIG. 16.7

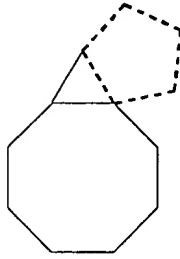
Goal: Create a five membered ring attached at the points shown.



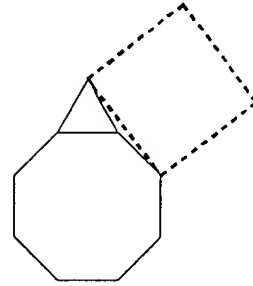
Attach regular
 \rightleftarrows
 polygon



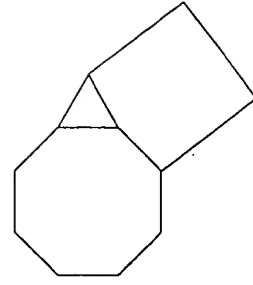
Attach regular
 \rightleftarrows
 polygon



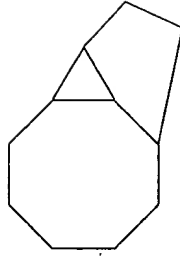
Use outer
 \rightleftarrows
 atoms



Final
 \rightleftarrows
 Result



Final
 \rightleftarrows
 Result



Final
 \rightleftarrows
 Result

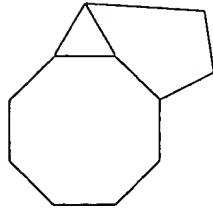
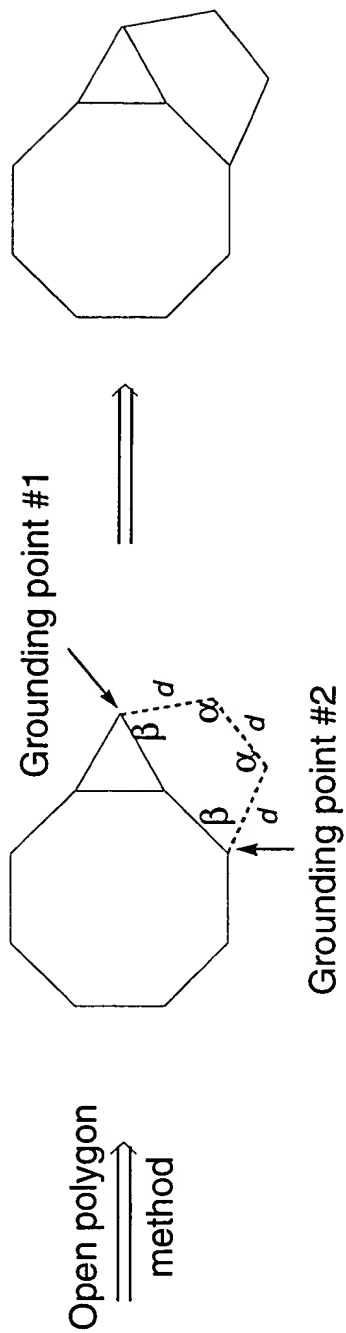
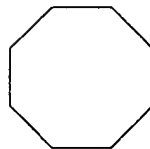



Fig. 8

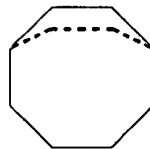


Goal: Create a five membered ring attached at the points shown.

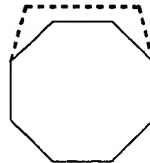
Fig. 9



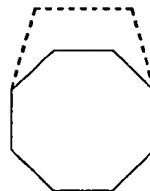
Attach a two-

 atom bridge



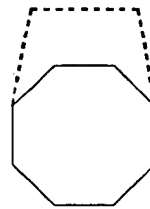
and



and



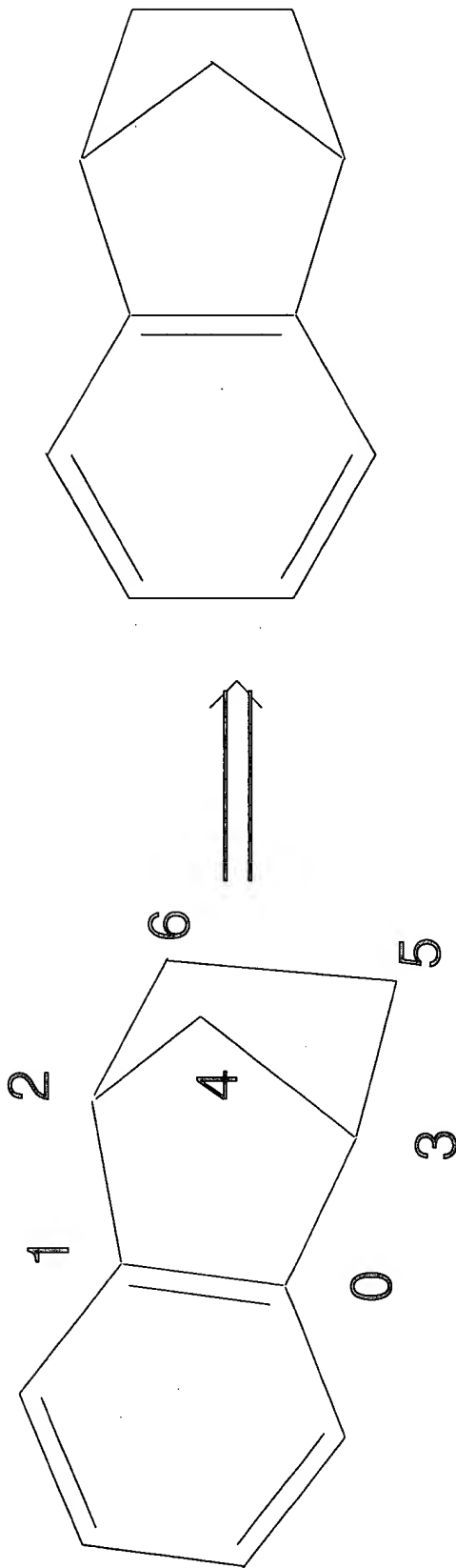
and



etc.

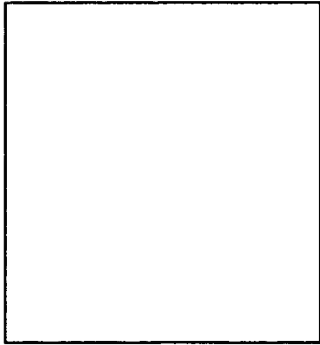
Fig. 10

If the bridge is not a ring, then the bridge is not a ring.
 If the bridge is not a ring, then the bridge is not a ring.
 If the bridge is not a ring, then the bridge is not a ring.

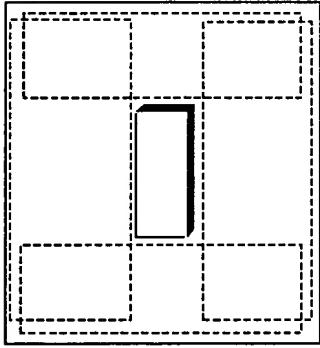


-----Enter RD_AttachPeeledBridge [3]
 Attaching peeled bridge at atoms 2 (CW) and 3 (CCW)
 Rating for bd len scale 1.0 is 198.294 (= congest[178.294] + BdLen[0.00] + bdAng[20 (bdAng=125)])
 Rating for bd len scale 0.5 is 313.185 (= congest[45.185] + BdLen[40.00] + bdAng[228 (bdAng=177)])
 Rating for bd len scale 0.7 is 291.643 (= congest[179.643] + BdLen[24.00] + bdAng[88 (bdAng=142)])
 Rating for bd len scale 0.9 is 242.107 (= congest[178.107] + BdLen[8.00] + bdAng[56 (bdAng=134)])
 Rating for bd len scale 1.1 is 93.917 (= congest[85.917] + BdLen[8.00] + bdAng[0 (bdAng=119)])
 Rating for bd len scale 1.3 is 56.154 (= congest[32.154] + BdLen[24.00] + bdAng[0 (bdAng=109)])
 Rating for bd len scale 1.5 is 61.044 (= congest[21.044] + BdLen[40.00] + bdAng[0 (bdAng=103)])
 Rating for bd len scale 1.7 is 72.576 (= congest[16.576] + BdLen[56.00] + bdAng[0 (bdAng=98)])
 Rating for bd len scale 1.9 is 86.400 (= congest[14.400] + BdLen[72.00] + bdAng[0 (bdAng=94)])
 Ring 1: Best bridge scale factor = 1.30 (rating = 56.154)
 Irregular polygon. (numAtsToDraw=4; RINGSIZ=5; aOuter_CW=2; _CCW=3)
 -----Exit RD_AttachPeeledBridge

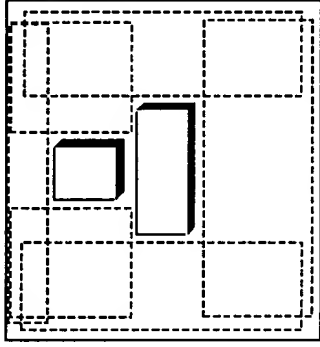
FIG. 11



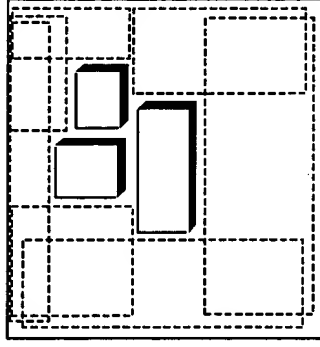
a. Initial free rectangle



b. After imprinting the first box, there are four free rectangles.

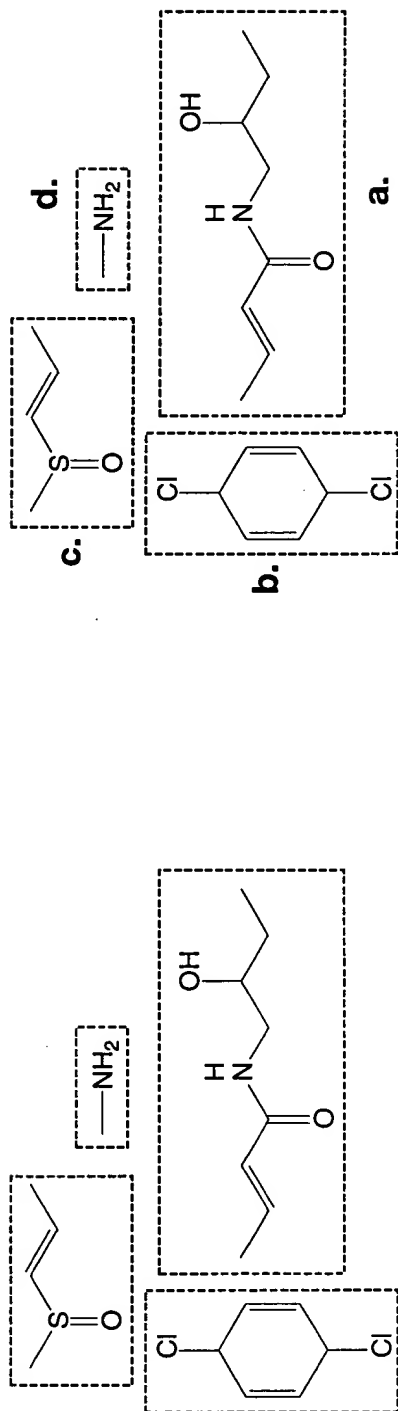


c. After imprinting the second box, there are seven free rectangles. (Translation step not included for clarity.)

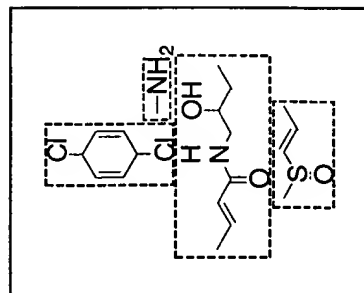


d. After imprinting the third box, there are eight free rectangles. (Translation step not included for clarity.)

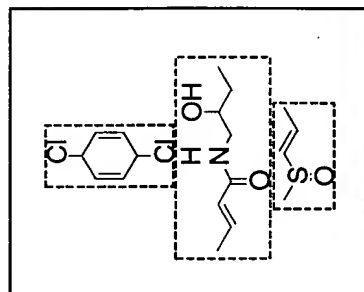
Fig. 12



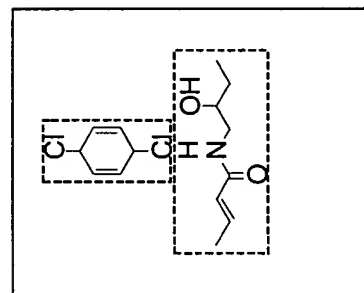
2. Boxes sorted by decreasing area.



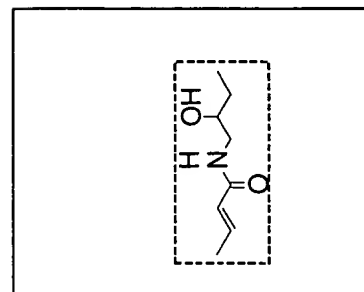
6. After placing fourth box.



5. After placing third box.



4. After placing second box.



3. After placing the largest box.

F16.13

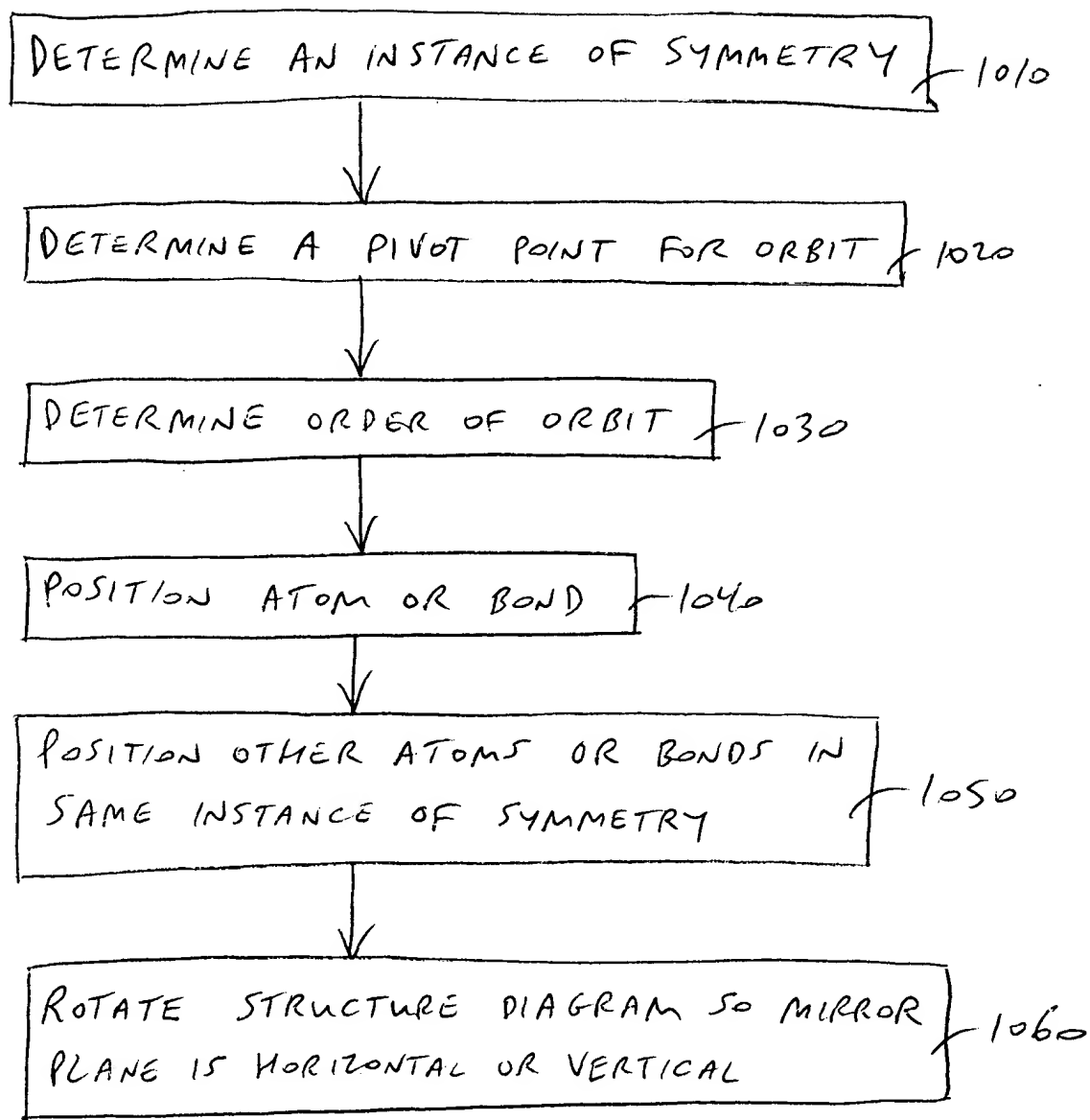


FIG. 14

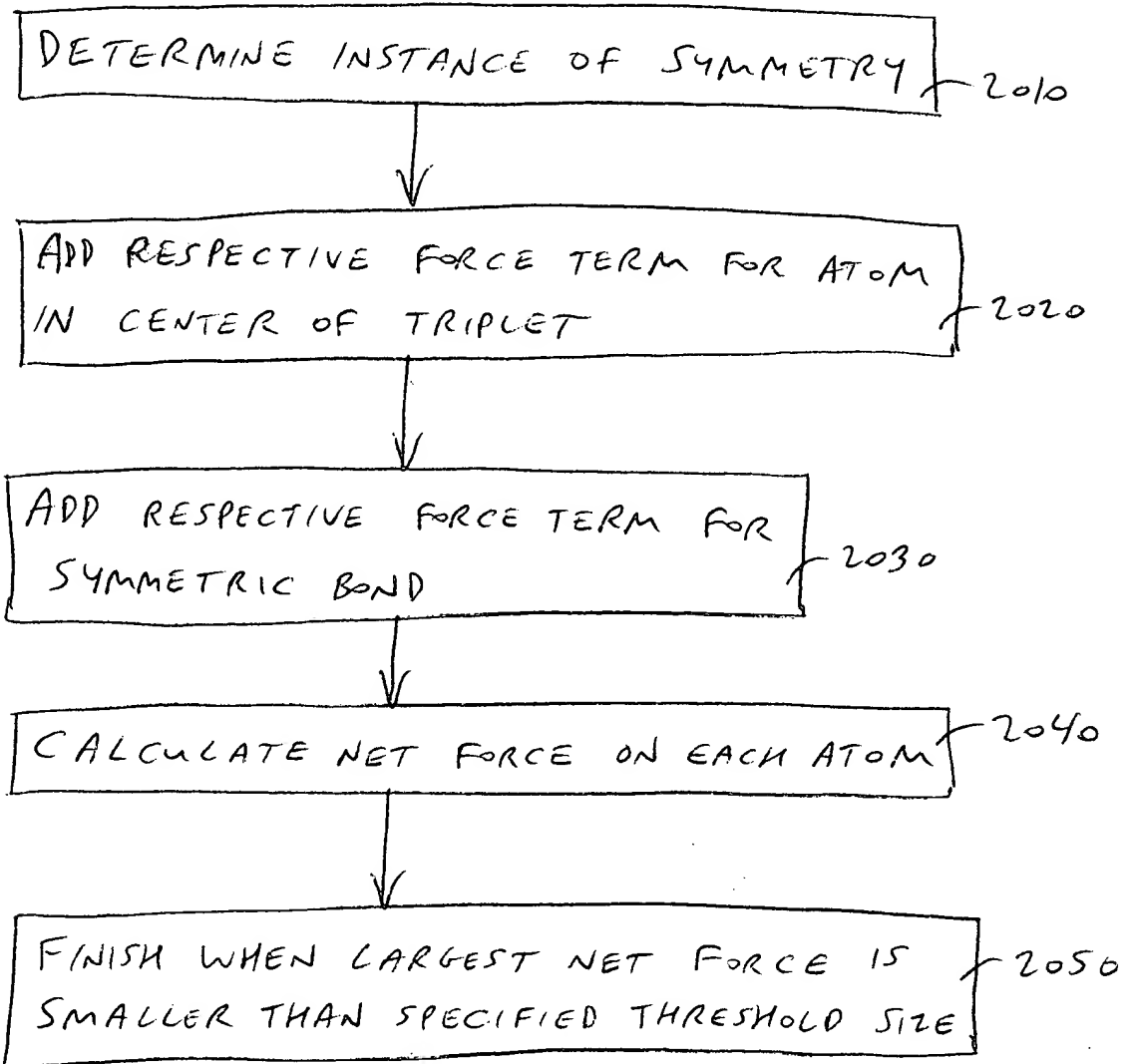


FIG. 15

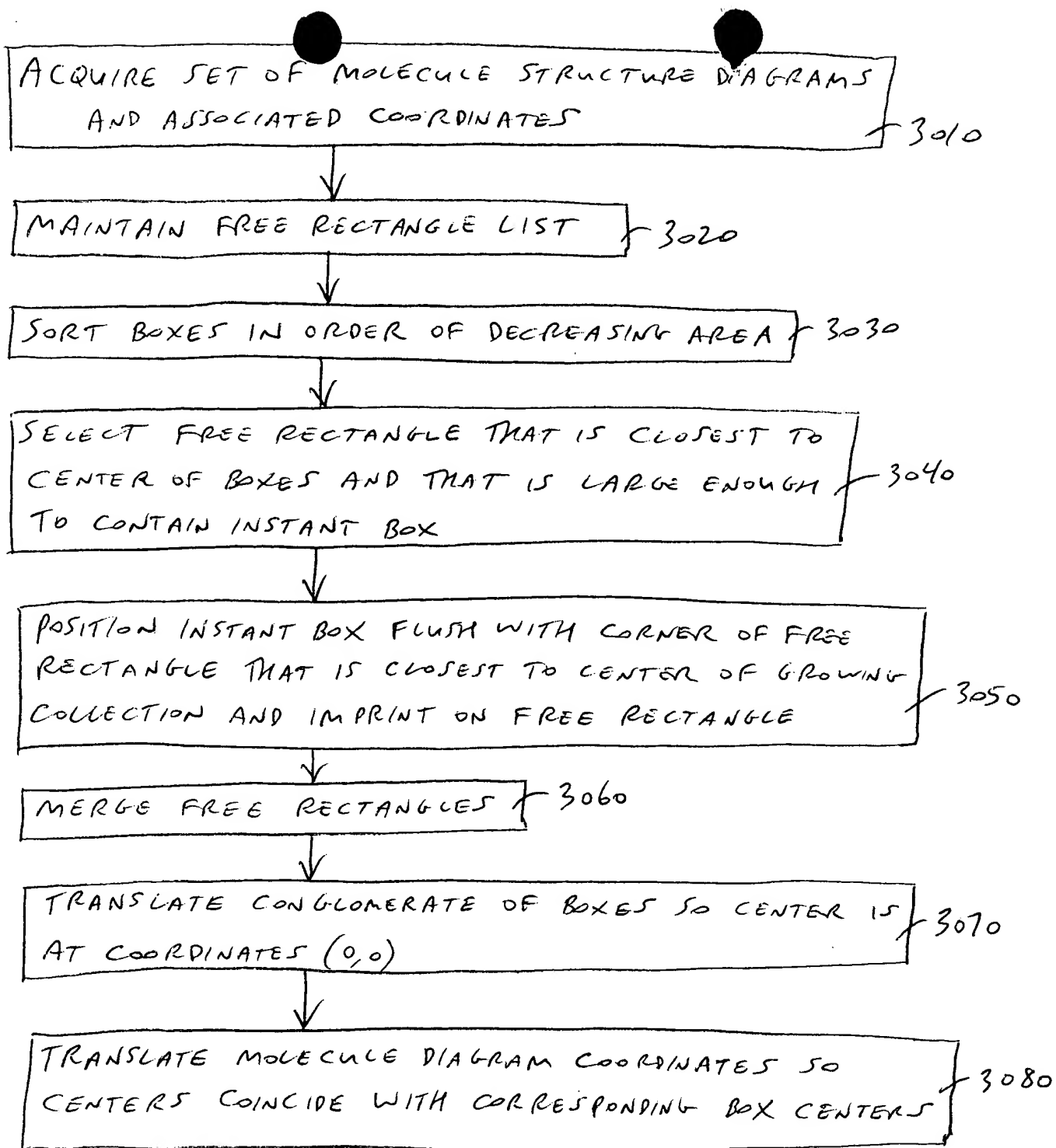


FIG. 16